Structure based drug design of some novel flavone derivatives.

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ABSTRACT

Computer-aided approaches have been widely used in pharmaceutical research to improve the efficiency of the drug discovery and development process. To identify and design small molecules as eligible drug candidates, various computational methods have been evaluated as promising strategies, depending on the purpose and systems of interest. Both ligand and structure-based drug design approaches are powerful technologies, which can be applied to lead identification and optimization. Here, in this present study, some novel flavones derivatives were synthesized and studied for structure based drug design to perform the studies based on the targets of interest. Computer aided structure based methods like Toxicity Risk assessment study (OSIRIS property calculator), Prediction of Activity Spectra for Substances (PASS), Rat acute toxicity prediction (GUSAR) and Molecular Docking (AC MECHO LEAD PRO VERSION 2.5) were done to accelerate the process and to minimize the synthetic and biological testing efforts. Structure Based Drug Design (SBDD) approach requires the understanding of receptor–ligand interactions. If the target 3D structure is known, it can be used for the design of new ligands. The structural information is either from X-ray crystallography, NMR, or from homology modeling. SBDD approaches are responsible for evaluating the complementarities and predicting the possible binding modes and affinities between small molecules and their macromolecular receptors. The Protein structure is collected from Protein Data Bank (PDB). Here some novel flavones derivatives are docked with Hexokinase (PDB ID-1V4S) for Antidiabetic Activity and Acetyl cholinesterase (PDB ID-1B41) for Nootropic (cognitive-enhancing) Activity and the free energy of binding in kcal/mol are compared with the standards.

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